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The viscosity to entropy ratio: from string theory motivated bounds to warm dense matter transport

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Abstract

We study the ratio of viscosity to entropy density in Yukawa one-component plasmas as a function of coupling parameter at fixed screening, and in realistic warm dense matter models as a function of temperature at fixed density. In these two situations, the ratio is minimized for values of the coupling parameters that depend on screening, and for temperatures that in turn depend on density and material. In this context, we also examine Rosenfeld arguments relating transport coefficients to excess reduced entropy for Yukawa one component plasmas. For these cases we show that this ratio is always above the lower-bound conjecture derived from string theory ideas.

Key words: viscosity; entropy density; Yukawa one-component plasmas; warm dense matter, self-diffusion
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1 Introduction

In 2005, Kovtun *et al.* (KSS)[1] conjectured from string theory arguments that in general, equilibrium media,

$$\frac{\eta}{s} \geq \frac{\hbar}{4\pi k_B}, \tag{1}$$

where η is the shear viscosity, s the entropy density, $\hbar$ the reduced Planck constant, and k_B the Boltzmann constant. This inequality is supposed to be valid for any finite-temperature relativistic quantum-field theory with zero chemical potential. Equality is obtained for theories with gravity duals, i.e., with anti de Sitter(AdS)/conformal field theory (CFT) correspondence. Given the speed of light does not appear, the inequality (1) could be true for non-relativistic systems. Kovtun *et al.*[1] further motivated their conjecture by showing data proving that (1) holds for common substances such as helium, nitrogen, or water. The inequality (1)can be examined for more exotic states of matter such as cold atomic gases or hot quark gluon plasmas (QGP)[2]. Indeed, the AdS/CFT correspondence finds applications in relativistic heavy-ion collisions in which QGP can be produced[3].

Thoma and Morfill[4] studied what happens to (1) in one-component plasmas (OCP)[5–8]. They have shown that inequality (1) is also valid for OCP, demonstrating that the ratio η/s is indeed minimized as function of the coupling parameter in strongly-coupled OCP when the thermal de Broglie length Λ is kept equal to the Wigner-Seitz radius d.

In this work, we extend the study of Thoma and Morfill[4] in two directions, to the case of the Yukawa screened OCP (YOCP)[8–16]. We also consider more realistic models of solid density materials in the warm dense matter (WDM) regime. We discuss the relevance of the Rosenfeld quasi-universal scaling law relating transport coefficients to excess reduced entropy in simple fluids[17,18]. The aim of this paper is to see what happens to the viscosity to entropy-density ratio in warm dense matter or screened strongly-coupled one-component plasmas.

2 YOCP

The YOCP are characterized by two parameters[16], i.e., the coupling parameter

$$\Gamma = \frac{(Ze)^2}{k_B T d} \tag{2}$$

and the screening parameter

$$\kappa = d/\lambda_D. \tag{3}$$

In these expressions, Z is the particle charge in units of elementary charge e, T the temperature, k_B the Boltzmann constant, and λ_D the screening length. This model considers a single type of particle of charge Ze in a polarizable charge-neutralizing background for which the screening property of the plasma is expressed by the Yukawa potential

$$\phi(R) = \frac{(Ze)e^{-R/\lambda_D}}{R}. \tag{4}$$

λ_D can be described by the Debye length, or more generally, by the finite-temperature Thomas-Fermi screening-length[19–21] which interpolates between the zero-temperature Thomas-Fermi screening-length and the Debye length.

The thermal de Broglie length $\Lambda = \sqrt{2\pi\hbar^2/mk_BT}$, where m is the mass of the plasma particles. The Wigner-Seitz radius d is related to the particle number density $n = N/V = 3/4\pi d^3$, where N is the particle number in the volume V. The plasma frequency $\omega_p = \sqrt{4\pi Z^2e^2n/m}$.

The ratio (1) involves two quantities, the shear viscosity η and the entropy density s. In our analysis, we usually consider a dimensionless viscosity

$$\eta^* = \frac{\eta}{mn\omega_p d^2}. \tag{5}$$

Care should be taken, given the various ways dimensionless viscosities appear in the literature. Fits exist for η^* as a function of Γ, κ that are deduced from molecular dynamic (MD) simulations[4,8]. One can show that $m\omega_p d^2 = \sqrt{3\Gamma} v_T dm$, where $v_T = \sqrt{k_BT/m}$ is the thermal velocity of the plasma particles. By definition, the entropy density $s = S/V$. In YOCP, we usually consider the dimensionless internal energy $u = U/Nk_BT$, free energy $f = F/Nk_BT$, and entropy $s^* = S/Nk_B$. U, F, and S are the internal energy, free energy, and entropy related by the thermodynamic relation $F = U - TS$ of the particle system. We consider only systems in thermodynamic equilibrium. Anticipating our application of the Rosenfeld scaling method, the normalized entropy s^* can be split into two parts, i.e., an ideal part s_{id}, and an excess part s_{ex}

$$s^* = s_{id} + s_{ex}. \tag{6}$$

The ideal part is given by[5]

$$s_{id} = \frac{5}{2} - \log n - 3\log\Lambda = \frac{5}{2} + \log(\frac{4\pi}{3}) - 3\log(\frac{\Lambda}{d}). \tag{7}$$

One can obtain s_{ex} as a function of Γ and κ using fits from MD simulations[9–13] or using the variational modified hypernetted chain (VMHNC) approach[22] applied to the YOCP[15]. One can show[4] that

$$k_B\frac{\eta}{s} = R(\Gamma,\kappa)v_T md, \tag{8}$$

where

$$R(\Gamma,\kappa) = \frac{\sqrt{3\Gamma}\eta^*}{s^*}. \tag{9}$$

Written in the form (8), one can see that $k_B\eta/s$ has the dimensions of an action, since $R(\Gamma,\kappa)$ is dimensionless. Indeed, if we express v_T and d in atomic units, one finds that $k_B\eta/s$ is proportional to $\hbar$. Then, the question concerns the value of this proportionality coefficient with respect to the string theory conjecture. It clearly depends on the system of interest. Note also that η^* and s^* depend on Γ and κ. Since we are considering a classical system of particles, $\Lambda < d$ leading to $v_T md > \sqrt{2\pi}\hbar$. If we use the lower limit that corresponds to $d = \Lambda$ in (8), the string theory limit (1) now reads

$$\sqrt{32\pi^3}R(\Gamma,\kappa) > 1. \tag{10}$$

We plot in Fig 1 the minimum of the left hand side of (10) as a function of Γ for various κ using the VMHNC[15], the Caillol-DeWitt[13,23], or the Hamaguchi[10,11,15] equations of state with a κ-dependent normalized-viscosity fit[8] or the VMHNC with a κ-independent normalized-viscosity fit[8]. We plot also results obtained using the hard-sphere Gibbs-Bogolyubov inequality (HS-GBI)[14]. When the fit of the normalized, i.e., dimensionless viscosity depends on the screening parameter κ (see Table IV in Ref.[8]), results does not depend on the equation of state used. However, we can see that using the fit independent of κ with $\kappa \leq 3$ can have a strong impact on results. This kind of fit should be used with caution. In any case, one can see that inequality (10) is obeyed. Our results are consistent with the one obtained by Thoma and Morfill[4] for OCP. They found 4.89 compared to values around 5. To be complete, we have also plotted results using the variational method based on the Gibbs-Bogolyubov inequality and the hard-sphere system to describe the YOCP[14]. The minimum ratio is a factor two above the previous results. This difference could be explained both by the approximate treatment of the equation of state using the Carnahan-Staring and Perkus-Yevick approximations and by the approximate estimation of the viscosity of OCP using the hard-sphere viscosity[14,16]. Note that the results are smooth and close to 10. Interestingly, this value is close to the values KSS show for helium, nitrogen, and water. Since in this example, we are on the boundary for which quantum effects may play a role, we are not so far from the string-theory lower-bound equal to one in our writing. This is one example of a situation for which the value of the minimum ratio is closer to the conjectured lower bound with the possible exception of the QGP[24]. For instance, in this reference, the minimum ratio was found to be roughly equal to 2π. Note finally that the existence of a minimum ratio is related to the one known for viscosity, which is a direct consequence of gas-like (atomic) to liquid-like (molecular) behavior[25,26] when Γ increases, i.e., when we consider the transition between weakly-coupled to a strongly-coupled YOCP.

3 Warm Dense Matter

One can also ask how the inequality (1) fares in more realistic warm dense matter models. As a first example, we plot in Fig 2 the normalized ratio $(4\pi k_B\eta)/(\hbar s)$ for liquid aluminum at density 2.37 g/cm^3 between 933 K and 20000 K using the HS-GBI method applied to the CPMD code[27]. 933 K corresponds to the melting point of aluminum at this density. We can see that the normalized ratio is minimum at $T_{Min} = 8000K$. The string theory bound is well satisfied. However, unlike the cases of the OCP and YOCP models, the minimum value is much larger, i.e, 123 vs. $\sim$ 10. It could be interesting to see what happens for hydrogen[28] or helium[29] near their metal-insulator transitions and for fluid lithium[30]. We expect the normalized ratio to be closer to one for these cases.

In Figures. 3 and 4, we plot T_{Min}, the normalized ratio $(4\pi k_B\eta)/(\hbar s)$, and Λ/d for hydrogen and helium as a function of density using the Thomas-Fermi method[31] to describe the ionization and the screening, i.e., the coupling and screening parameters, and the HS-GBI to get viscosity and entropy using the same method as for YOCP. T_{Min} is the temperature obtained when the normalized ratio is minimum. In fact, the Thomas-Fermi approach allows ourselves to describe WDM as effective YOCP. As expected, we are closer to one by considering these two elements, hydrogen being the closest. These are densities of interest for inertial confinement fusion[32]. The minimum temperature increases with density, whereas the normalized ratio shows a maximum at 5.36 g/cm^3 ($T_{Min} = 0.89$ eV and normalized ratio equal to 12.02) for hydrogen, and 41.12 g/cm^3 ($T_{Min} = 3.97$ eV and normalized ratio equal to 28.22) for helium. In any case, the string-theory bound is satisfied, but one may wonder what happens for hydrogen if we keep on compressing it to see how we match with results from nuclear theory. This kind of study is a real example of research that can mix various parts of usually uncorrelated domains of physics. This is a strong indicator of its fruitfulness. Concerning the ratio Λ/d, we can see that in both cases, it is lower that one and there is a minimum reached at 5.51 g/cm^3 ($T_{Min} = 0.89$ eV and $\Lambda/d = 0.41$) for hydrogen and 42.66 g/cm^3 ($T_{Min} = 4.07$ eV and $\Lambda/d = 0.12$) for helium. Normalized ratio maximum and Λ/d ratio minimum are clearly related. Again, the quantum character of hydrogen is more significative than the helium one since the ratio Λ/d is the largest for hydrogen for the studied cases.

4 Rosenfeld method for YOCP

A very interesting result can be found if we consider again the YCOP and the Rosenfeld quasi-universal scaling law relating transport coefficients to excess reduced entropy in simple fluids[17,18]. From Eq. (7), one can see that if $d = \Lambda$, the entropy of the ideal gas is constant. For dilute and dense simple fluids, shear viscosity and self-diffusion depend only on the excess reduced entropy s_{ex} when properly normalized[18]. The normalized ratio reads[18]

$$\frac{4\pi k_B \eta}{s\hbar} = \frac{2^{19/6}\pi^{11/6}}{3^{1/3}} \frac{0.2e^{0.8\tilde{s}}}{\frac{5}{2} + \log(\frac{4\pi}{3}) - \tilde{s}} \tag{11}$$

for dense fluids ($\tilde{s} > 1$, freezing is obtained when $4 < \tilde{s} < 5$), and

$$\frac{4\pi k_B \eta}{s\hbar} = \frac{2^{19/6}\pi^{11/6}}{3^{1/3}} \frac{0.27\tilde{s}^{-2/3}}{\frac{5}{2} + \log(\frac{4\pi}{3}) - \tilde{s}} \tag{12}$$

for dilute fluids ($\tilde{s} < 0.1$, the ideal gas is for $\tilde{s} = 0$). We introduced $\tilde{s} = -s_{ex}$ for simplicity. The consequence of this scaling is very interesting because we can see that the normalized ratio is minimum for some nearly universal $\tilde{s}_0$. As an illustration, we have chosen a simple cubic polynomial interpolation of the logarithm of the normalized ratio using $\tilde{s}$ as a variable between $\tilde{s} = 0.1$ and $\tilde{s} = 1$, i.e., in the domain that makes the transition between dilute to dense fluids. One finds that $\tilde{s}_0 = 0.546$ and the corresponding normalized ratio is equal to 4.84. This value is very close to the one found by Thoma and Morfill[4] for OCP, i.e., 4.89, and to what has been obtained in Fig. 1 with Caillol-DeWitt, Hamaguchi, or VMHNC cases. Note that if we use $s_{ex} = -0.546$ for OCP[4], one finds that the minimum is obtained for $\Gamma = 4.95$ which differs notably from the value of $\Gamma = 12$ previously obtained by Thoma and Morfill[4]. Though approximate, the approach of Rosenfeld in the case of YCOP is rather remarkable because the coupling and screening parameters disappear completely when $d = \Lambda$. This approach can really be called quasi-universal. As an illustration, we plot in Fig. 5 the normalized ratio as a function of minus the excess reduced entropy to show how this quasi universal curve looks as well as a cubic polynomial interpolation matches with dense and dilute domains. Since we are assuming that $d = \Lambda$, note that the ratio becomes singular for $\tilde{s} = 5/2 + \log(4\pi/3)$. It is also singular for the ideal gas, i.e., when $\tilde{s} = 0$. In Fig. 6 we plot the ratio of Γ to Γ_{mel} as a function of κ, where Γ_{mel} is the value of Γ at the fluid-solid phase-transition[11,8] and Γ is such that $s_{ex}(\Gamma, \kappa) = -0.546$ using VMHNC. For comparison, we give (diamonds) the value of Γ/Γ_{mel} for the case VMHNC encountered in Fig. 1. For the cases studied, $\Gamma/\Gamma_{mel} \approx 0.03$ when $s_{ex}(\Gamma, \kappa) = -0.546$. It is more erratic for diamonds. Additional viscosity fits as a function of κ could be helpful.

Up to now for YOCP, we have examined what happens when $d = \Lambda$. It is possible to extend this study at fixed $\Lambda/d < 1$. The only change is to divide the normalized ratio by Λ/d while still using Eq. (7). As an illustration, we plot in Fig 7 what happens to $\tilde{s}_0$ and the corresponding normalized ratio as a function of $\Lambda/d < 1$. One can see that $\tilde{s}_0$ does not vary too much, being a decreasing function of Λ/d. On the contrary, the variation of the normalized ratio is far more important, being a decreasing function of Λ/d too. As expected, the smaller Λ/d is, the more classical the system is. It could be interesting to extend this study in the quantum regime where $\Lambda/d > 1$ to see what happens to the normalized ratio. This is not easy because we need then an equation of state and transport coefficients for interacting many-particle quantum systems[33–35].

5 Conclusion

We have shown that the ratio of the viscosity to the entropy density satisfied the KSS lower bound conjecture in screened strongly coupled plasmas and realistic warm dense matter models with typical values of $(4\pi k_B \eta)/(\hbar s) \sim 10$ to 100. No violation of the string-theory lower-bound was found for YOCP or the WDM cases that were considered. The string theory lower-bound also was found to combine remarkably with the Rosenfeld quasi-universal scaling law to predict a unique value of -0.546 for the reduced excess entropy at the minimum ratio point.

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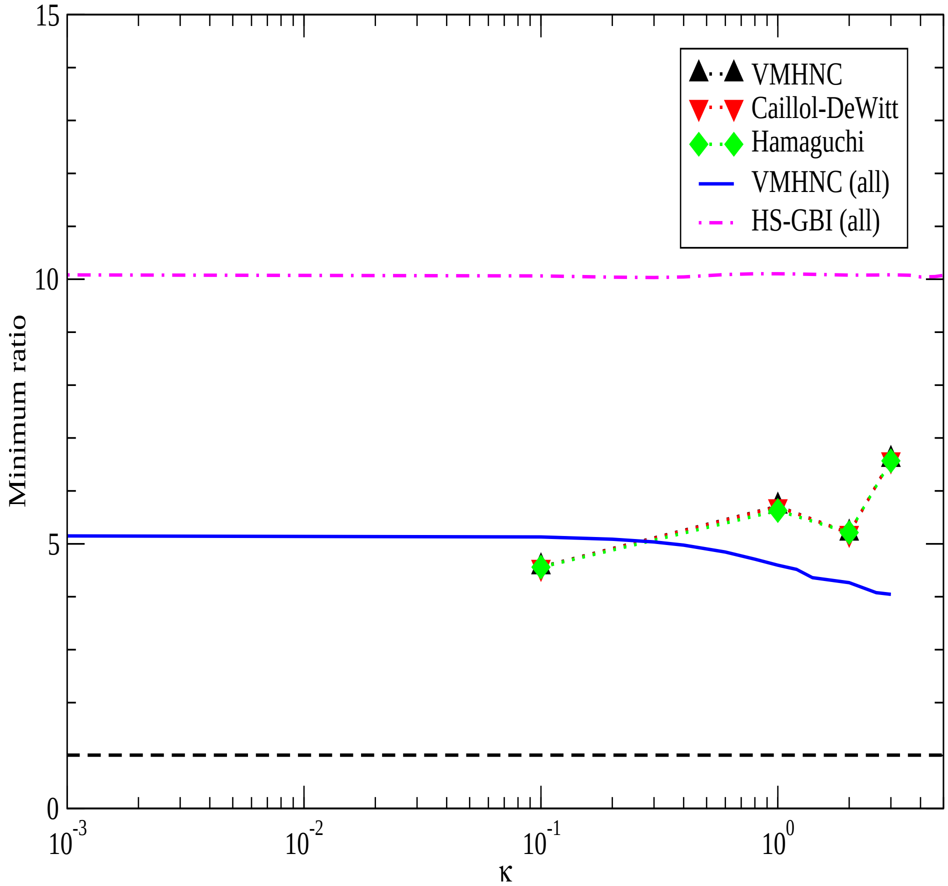

Fig. 1. (Color on line) Minimum ratio as a function of screening parameter κ using the VMHNC[15], the Caillol-DeWitt[13,23], or the Hamaguchi[10,11,15] equation of state with a κ-dependent normalized-viscosity solid-density aluminum[8]. We plot also results obtained using the hard-sphere Gibbs-Bogolyubov inequality (HS-GBI)[14] or the VMHNC with a κ-independent normalized-viscosity fit[8] (all). The dashed-line is the string-theory lower-bound equal to one.

FIGURE 1

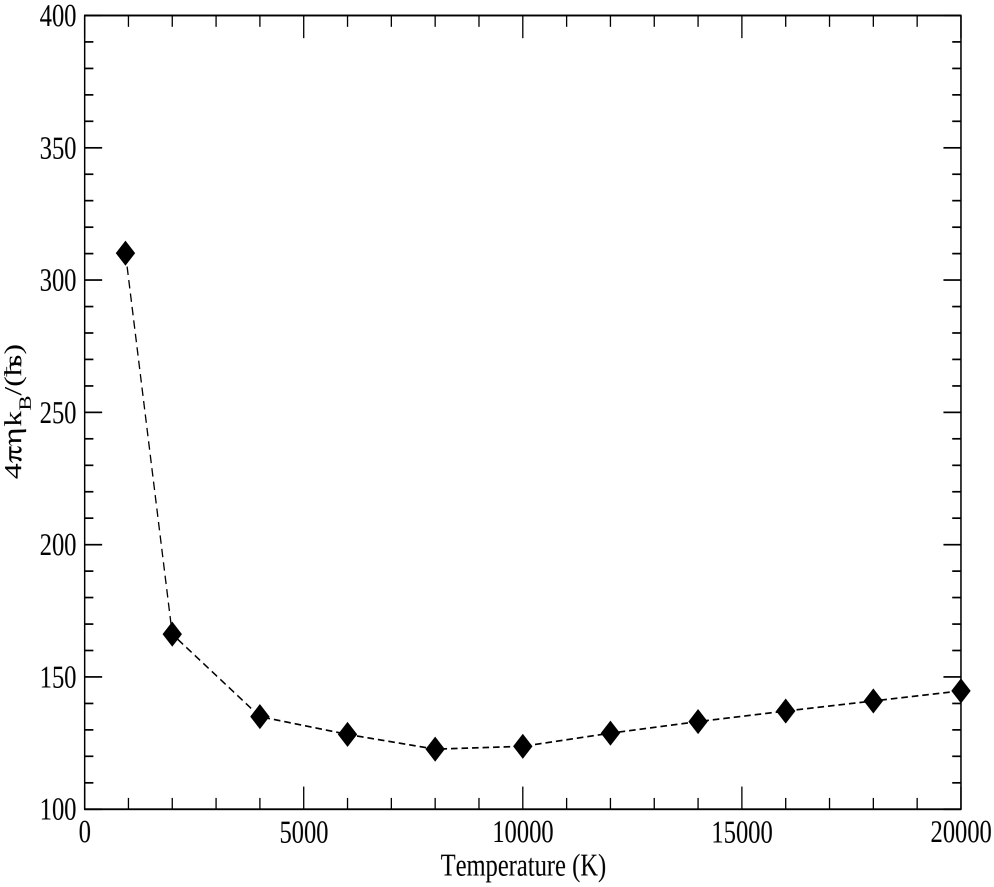

Fig. 2. Normalized ratio $(4\pi k_B \eta)/(\hbar s)$ as a function of temperature for liquid-density aluminum using the HS-GBI method applied to the CPMD code[27].

FIGURE 2

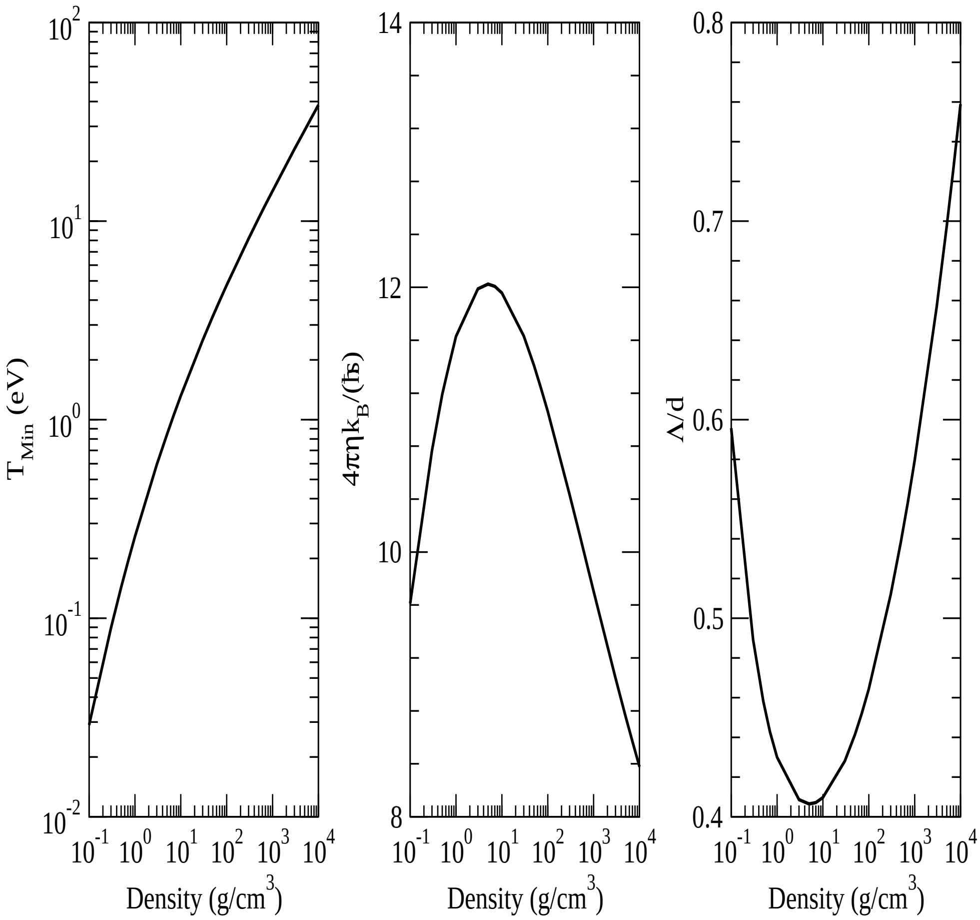

Fig. 3. Minimum temperature T_{Min}, normalized ratio $(4\pi k_B \eta)/(\hbar s)$, and Λ/d for hydrogen as a function of density. The Thomas-Fermi HS-GBI has been used to estimate the minimum temperature and the normalized ratio.

FIGURE 3

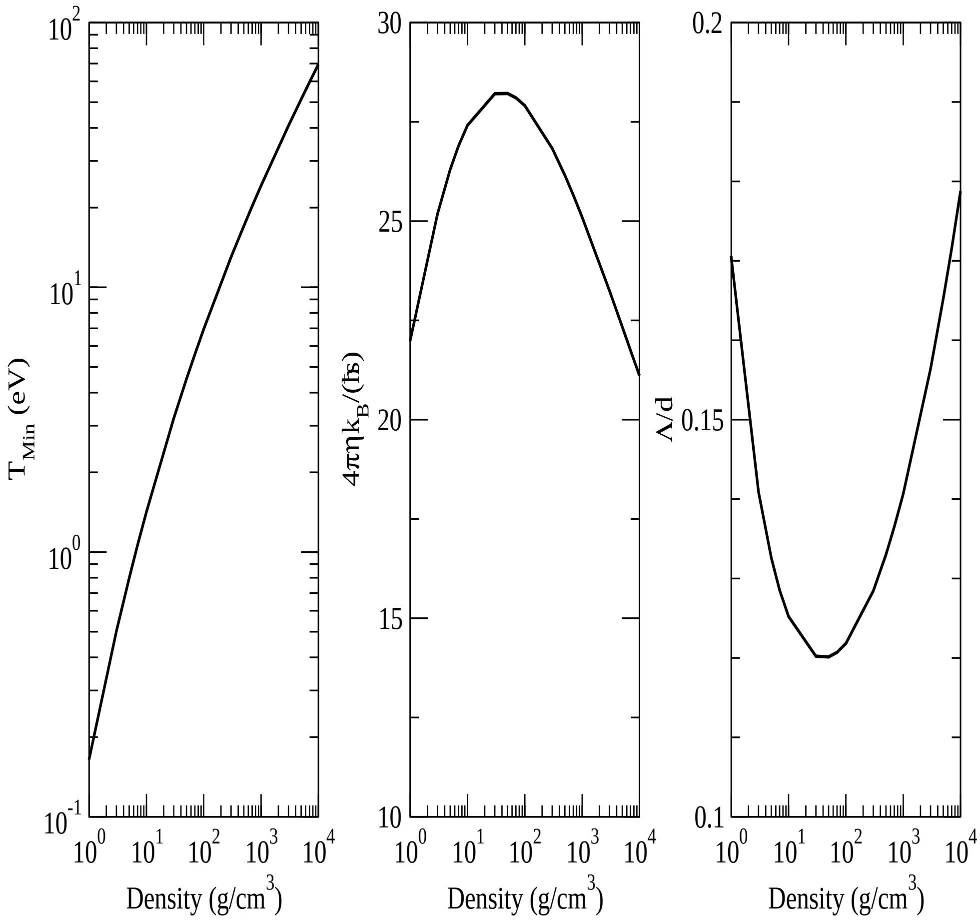

Fig. 4. Minimum temperature T_{Min}, normalized ratio $(4\pi k_B \eta)/(\hbar s)$, and Λ/d for helium as a function of density. The Thomas-Fermi HS-GBI has been used to estimate the minimum temperature and the normalized ratio.

FIGURE 4

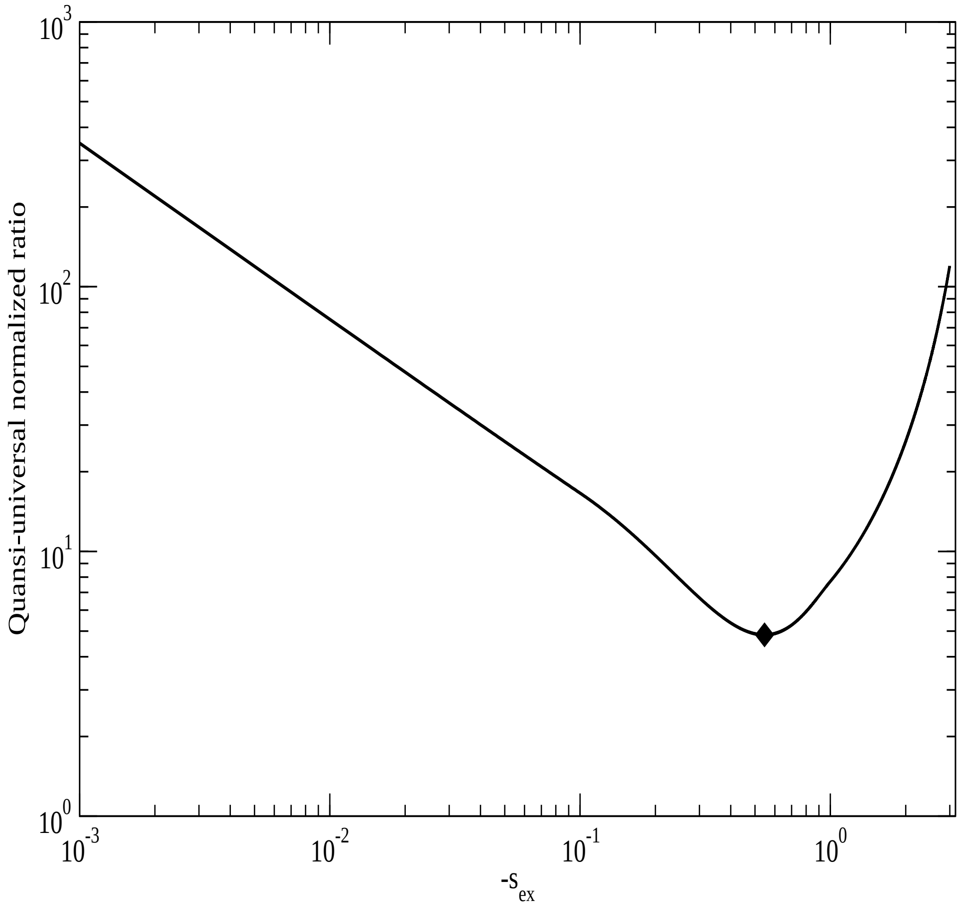

Fig. 5. Quasi-universal normalized ratio as a function of minus the excess reduced entropy for YOCP. The diamond indicates the minimum 4.84 located at $s_{ex} = -0.546$.

FIGURE 5

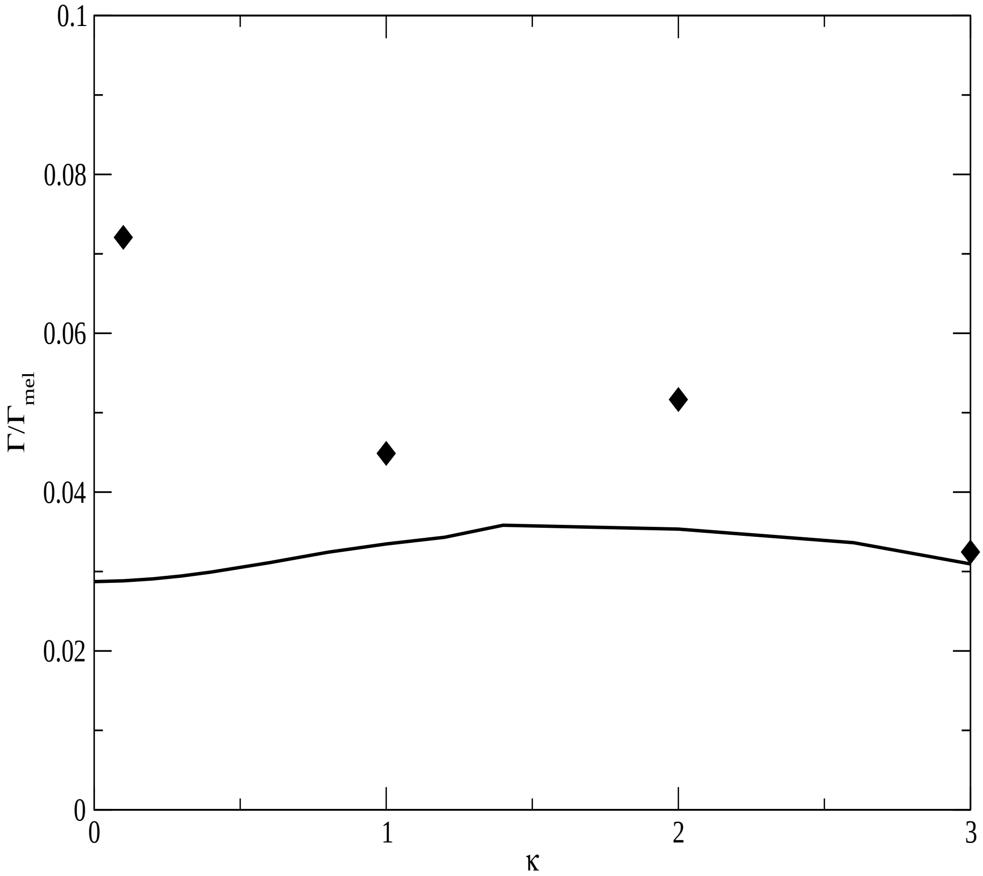

Fig. 6. Ratio of Γ, such that $s_{ex}(\Gamma, \kappa) = -0.546$ using VMHNC, to Γ at the fluid-solid phase-transition[11,8] as a function of the screening parameter κ (for diamonds see text).

FIGURE 6

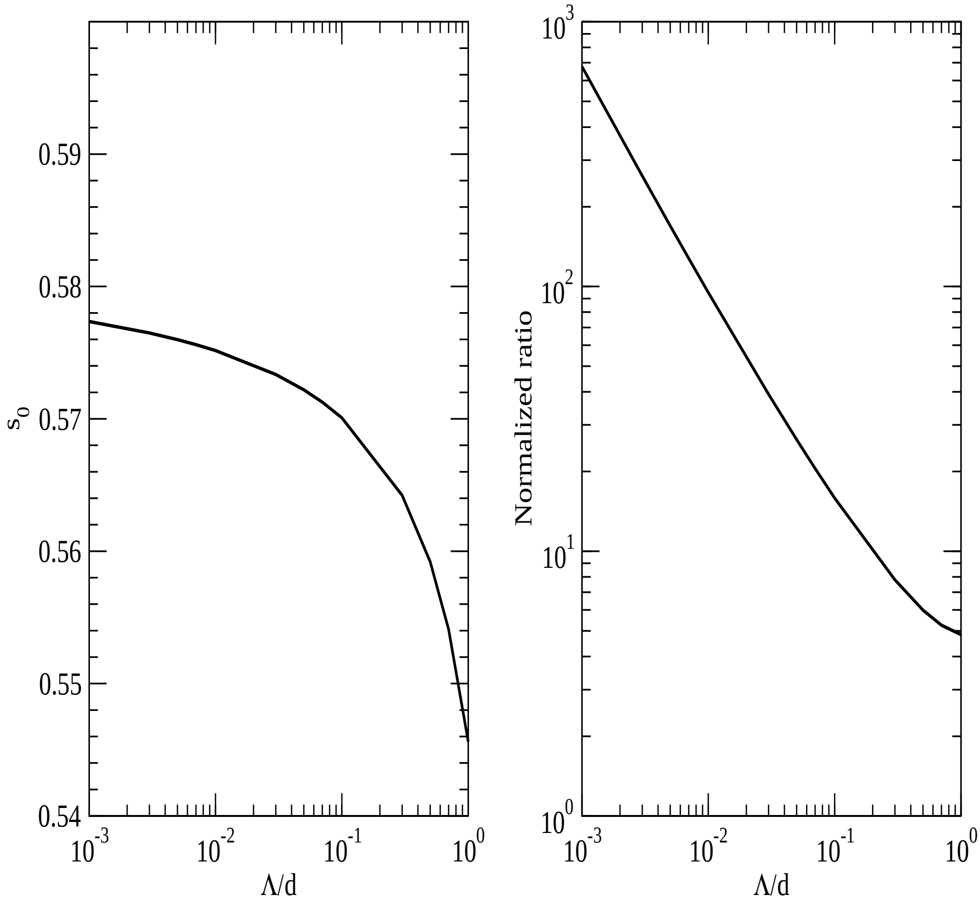

Fig. 7. Quasi-universal $\tilde{s}_0$ and normalized ratio as a function of Λ/d.
FIGURE 7